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STUDIES OF ELECTRONIC AND STRUCTURAL INTERACTIONS AT
SURFACES: METAL OVER. (U) MINNESOTA UNIV MINNEAPOLIS
DEPT OF CHEMICAL ENGINEERING AND M. J H WEAVER

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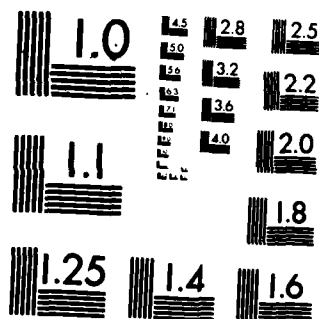
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Final Report

(Award dates: 1 September 1983 through 31 August 1986)

for

**Studies of Electronic and Structural Interactions at Surfaces:
Metal Overlayers on Semiconductors**

John H. Weaver

**Department of Chemical Engineering and Materials Science
University of Minnesota
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Part I

a. Papers Submitted to Refereed Journals (and not yet published)

1. M.W. Ruckman, J.J. Joyce, F. Boscherini, and J.H. Weaver, "Ga and As Interdiffusion and Reaction at Fe/GaAs(110) and Co/GaAs(110) Interfaces," J. Vac. Sci. Technol.
2. J.J. Joyce and J.H. Weaver, "Characterization of an Extended Reactive Noble-Metal/III-V Semiconductor Interface: Cu/GaAs(110)," Proceedings of the Materials Research Society.
3. M. del Giudice, R.A. Butera, J.J. Joyce, M.W. Ruckman, and J.H. Weaver, "Temperature Dependent Intermixing at the V/Ge(111) Interface," Proceedings of the Materials Research Society.

b. Papers Published in Refereed Journals

4. J.H. Weaver, "Interface Research: Reactions at Metal/Semiconductor Boundaries," *Physics Today*, January 1986, pp. 24-26 and cover photo.
5. M.W. Ruckman, J.J. Joyce, and J.H. Weaver, "Interdiffusion and Reaction at the Fe/GaAs(110) Interface," *Phys. Rev. B* 33, 7029-7035 (1986).
6. M. del Giudice, R.A. Butera, M.W. Ruckman, J.J. Joyce, and J.H. Weaver, "V/Ge(111): Temperature Dependent Intermixing Studied with High Resolution Photoemission and Quantitative Modeling," *J. Vac. Sci. Technol. A* 4, 879-881 (1986).
7. M. Grioni, J.J. Joyce, and J.H. Weaver, "Metal-Anion Bond Strength and Room Temperature Diffusion at Metal/GaAs Interfaces: Transition versus Rare-Earth versus Au Metal Overlayers," *J. Vac. Sci. Technol. A* 4, 965-968 (1986).
8. A. Fujimori, M. Grioni, and J.H. Weaver, "Rare-Earth-Metal/Semiconductor Interfacial Reactions: Thermodynamic Aspects," *Phys. Rev. B* 33, 726-735 (1986).
9. M.W. Ruckman, M. del Giudice, J.J. Joyce, and J.H. Weaver, "Photoemission Study of the Development of the Ti/GaAs(110) Interfaces," *Phys. Rev. B* 33, 2191-2197 (1986).
10. M. del Giudice, M. Grioni, J.J. Joyce, M.W. Ruckman, S.A. Chambers, and J.H. Weaver, "Modeling Homogeneous and Heterogeneous Metal/Semiconductor Interface Reactions with Photoemission using Angle Resolved Auger Spectroscopies," *Surf. Sci.* 168, 309-322 (1986).
11. R.A. Butera, M. del Giudice, and J.H. Weaver, "Quantitative Modeling of Reactive Metal/Semiconductor Interface Growth using High Resolution Photoemission Results," *Phys. Rev. B* 33, 5435-5449 (1986).
12. J.H. Weaver, M. Grioni, and J.J. Joyce, "Critical Development Stages for the Reactive Cr-GaAs(110) Interface," *Phys. Rev. B* 31, 5348-5354 (1985).
13. J.H. Weaver, M. Grioni, J.J. Joyce, and M. del Giudice, "Reactions at a Rare-Earth/GaAs Interface: Ce/GaAs," *Phys. Rev. B* 31, 5290-5296 (1985).

14. M. Grioni, M. del Giudice, J.J. Joyce, and J.H. Weaver, "Modeling of Interface Reaction Products with High Resolution Core Level Photoemission," J. Vac. Sci. Technol. A3, 907-910 (1985).
15. M. Grioni, J.J. Joyce, and J.H. Weaver, "Reaction at a Refractory-Metal/Semiconductor Interface: V/GaAs(110)," J. Vac. Sci. Technol. A3, 918-921 (1985).
16. M.W. Ruckman, M. del Giudice, and J.H. Weaver, "Temperature Dependent Growth Morphology of a Semiconductor/Metal Interface: Ge/Ta(110)," Phys. Rev. B 32, 1077-1084 (1985).
17. M. Grioni, J.J. Joyce, and J.H. Weaver, "Adatom Aggregation, Reaction, and Chemical Trapping at the Sm/GaAs(110) Interface," Phys. Rev. B 32, 962-968 (1985).
18. M. del Giudice, J.J. Joyce, M.W. Ruckman, and J.H. Weaver, "Cluster Formation and Atomic Intermixing at the Reactive V/Ge(111) Interface," Phys. Rev. B 32, 5149-5155 (1985).
19. A. Franciosi, P. Perfetti, A.D. Katnani, J.H. Weaver, and G. Margaritondo, "Samarium Chemisorption on Group-IV Semiconductors," Phys. Rev. B 29, 5611-5616 (1984).

c. **Books (and sections thereof) Submitted for Publication**

20. J.H. Weaver, "Synchrotron Radiation Studies of Surfaces and Interfaces," Chapter 4 in *Analysis and Characterization of Thin Films*, edited by K.N. Tu and R. Rosenberg (Academic Press, NY) (jointly supported by Army Research Office and Minnesota's Microelectronic and Information Sciences Center)

d. **Books (and sections thereof) Published**

None

e. **Patents Filed**

None

f. **Patents Granted**

None

g. **Invited Presentations at Topical or Scientific/Technical Society Conferences**

1. J.H. Weaver, "Reactions at Metal/Semiconductor Interfaces," Materials Research Society Meeting, Boston, MA, December 1986.
2. J.H. Weaver, Session Chairman, Session on Epitaxial Growth II, National Symposium of the American Vacuum Society, Baltimore, MD, October 1986.
3. J.H. Weaver, Stanford Workshop on III-V's, Stanford, CA, October 1986.
4. J.H. Weaver, "High Resolution Photoemission Studies of Reactive Metal/Semiconductor Interfaces," International Workshop on Physics of Interfaces by Synchrotron Radiation and Other High Energy Probes, Bad Honnef, West Germany, April 1986.

5. J.H. Weaver, "High Resolution Core Level Photoemission of Interfaces," Workshop on an Advanced Soft X-Ray and Ultraviolet Synchrotron Source, Berkeley, CA, November 1985.
6. J.H. Weaver, "Materials Science of Complex Systems: Microelectronics," Control Data High Technology Futures Workshop, Minneapolis, MN, October 1985.
7. J.H. Weaver, "Modeling Homogeneous and Heterogeneous Metal/Semiconductor Interface Reactions with Photoemission and Angle-Resolved Auger Spectroscopies," International Conference on the Formation of Semiconductor Interfaces, Marseilles, France, June 1985.
8. J.H. Weaver, "Metal Semiconductor Reactions," MEIS Workshop on New Frontiers in Semiconductor Materials, University of Minnesota, Minneapolis, MN, August 1984.
9. J.H. Weaver, "Synchrotrons and Materials Science Research: VUV Applications," an address to the DEPTH Committee, AIME/ASM, Detroit, MI, September 1984.

h. Contributed Presentations at Topical or Scientific/Technical Society Conferences

1. J.J. Joyce, M. Grioni, M. del Giudice, F. Boscherini, M.W. Ruckman, and J.H. Weaver, "Quantitative Modeling of Metal/GaAs(110) Interface Formation using High Resolution Core Level Photoemission," 33rd National Symposium of the American Vacuum Society, Baltimore, MD, October 1986.
2. S.A. Chambers, D.M. Hill, F. Xu, M. del Giudice, and J.H. Weaver, "Determination of Diffusion Parameters for Silicide Formation at the Ti/Si(111) Interface," 33rd National Symposium of the American Vacuum Society, Baltimore, MD, October 1986.
4. J.H. Weaver, "Modeling Metal/Semiconductor Interfaces with Synchrotron Radiation Photoemission," IBM Watson Research Center, Yorktown Heights, NY, May 1985.
5. M. Grioni, J.J. Joyce, and J.H. Weaver, "Reaction at a Refractory Metal/Semiconductor Interface: V/GaAs(110)," 31st National Symposium of the American Vacuum Society, Reno, Nevada, December 1984.
6. M. Grioni, M. Del Giudice, J.J. Joyce, and J.H. Weaver, "Modeling of Interface Reaction Products with High Resolution Core Level Photoemission," 31st National Symposium of the American Vacuum Society, Reno, Nevada, November 1984.
7. M. Grioni, J.J. Joyce, and J.H. Weaver, "Electronic Structure and Interface Chemistry of Reactive Rare Earth/III-IV Semiconductor Junctions: Ce/GaAs(110)," 17th Annual Synchrotron Radiation Center Users Group Meeting, Stoughton, Wisconsin, October 1984.
8. J.J. Joyce, M. Grioni, and J.H. Weaver, "Critical Stages in the Development of the Cr/GaAs(110) Interface," 17th Annual Synchrotron Radiation Users Group Meeting, Stoughton, Wisconsin, October 1984.
9. J.H. Weaver, "Metal/Semiconductor Interfaces," Research Frontiers Lecture, Honeywell Corporate Technology Center, Minneapolis, MN, September 1984.

ONR Final Report
Grant N00014-83-K-0579
J.H. Weaver, PI

10. J.H. Weaver, "Reactions at Metal Semiconductor Interfaces," MEIS III-V Seminar, Minneapolis, MN, May 1984.
11. J.H. Weaver, "Metal Overlayers on Semiconductors," Colloquium, Department of Physics, Iowa State University, Ames, IA, February 1984.

i. **Honors/Awards/Prizes**

John J. Joyce, Materials Research Society 1985 Student Award

John H. Weaver, 1986 George Taylor/IT Alumni Society Research Award, University of Minnesota

John J. Joyce, Nominee for the 1986 M.M. Traum Award to be presented at the American Vacuum Society, Baltimore, MD, October 1986.

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Part II

a. Funding history

John H. Weaver, Principal Investigator

Studies of Electronic and Structural Interactions at Surfaces: Metal Overlayers on Semiconductors. Starting date 1 September 1983. 36 month duration

Year 1 -- 1 September 1983 - 31 August 1984: \$81,009

Year 2 -- 1 September 1984 - 31 August 1985: \$89,995

equipment supplement for small spot x-ray photoelectron spectrometer: \$101,700

Year 3 -- 1 September 1985 - 31 August 1986: \$98,779

b. Cognizant ONR Scientific Officer: David Nelson

c. Current telephone number: (612) 625-6548

d. Project description

We have examined the electronic interactions and structural modifications which occur when metal overlayers are deposited onto clean semiconductor surfaces. We have examined these interactions as the physical and chemical parameters of the surface/interface are changed, have assessed atomic interdiffusion and overlayer reaction, and have determined whether clusters form and how they affect the properties of the interface. We have sought fundamental information describing interface evolution from the initial adatom on a surface through the growth of the extended, fully-reacted, microscopic interface.

e. Significant results

In Part I, we list 20 refereed papers that have come from this program, together with the invited papers, contributed papers, and awards. A brief synopsis of our work follows:

We have been able to show that reactions at surfaces are highly heterogeneous, both parallel and perpendicular to the surface. The degree of lateral heterogeneity varies with the details of the initial interactions of atoms on the surface, with epitaxy observed in some cases (e.g. Fe/GaAs and Co/GaAs) and microcrystallites in others (e.g. Ti/GaAs, Au/GaAs, Ce/GaAs, V/Ge). We have examined the thermochemistry of these reactions, applying bulk concepts where possible and investigating the limits of bulk thermodynamics. We have made significant progress in understanding the reaction products themselves by advancing the state-of-the-art of high resolution synchrotron radiation photoemission and using that technique to investigate chemical shifts. These core level studies have lead to a much improved picture of heterogeneity perpendicular to the surface. In particular, we have shown that well defined and distinct chemical phases form at interfaces, even though the spatial extent of the interface is only a few atomic layers. These layers can be polycrystalline or single crystal, and the morphology that they exhibit determines the scale over which they form. Room temperature studies have shown the formation of very narrow, metastable germanides or arsenides whose properties enhance or restrict further atomic intermixing. We have been able to demonstrate that subsequent interface growth gives rise to second phases which resemble compounds in some cases or solid solutions in others. With this chemical information, we believe we have developed general pictures for interface formation. We have then taken the next step of seeking to quantitatively model these interfaces. These quantitative models, as they are further developed, will ultimately lead to predictive capabilities. Finally, we have

undertaken investigations of the temperature dependence of interfaces, testing our room temperature models and extending the limits of our mathematical modeling. These studies, and the complementary work done elsewhere as a result of the scientific leadership of our laboratory, will have a major impact on the way interface research is done and the development of the discipline.

f. Graduate students and post-doctorals

John H. Weaver, PI
Richard A. Butera, Visiting Professor
Marco Grioni, Postdoc
Massimo del Giudice, Postdoc
Mark W. Ruckman, Postdoc
John J. Joyce, PhD student

g. Technical reports

Technical reports 1-20 have been submitted to ONR during the grant period.

END

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